

1,3-Benzodioxole-5-methanol
495-76-1 | DTXSID3060089

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 3.86e-01

Global applicability domain: Inside

Local applicability domain index: 6.21e-01

Confidence level: 7.39e-01

Nearest Neighbors from the Training Set

Image not found

1,3-Benzodioxole-5-methanol

Measured: 1.05

Predicted: 3.86e-01

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Maltol

Measured: 0.09

Predicted: -0.0719

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4H-Pyran-4-one, 5-hydroxy-2-methyl-

Measured: -0.590

Predicted: -0.250

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2-Ethyl-3-hydroxy-4H-pyran-4-one

Measured: 0.63

Predicted: 4.56e-01